Variants of symmetry-based indicators in the band theory

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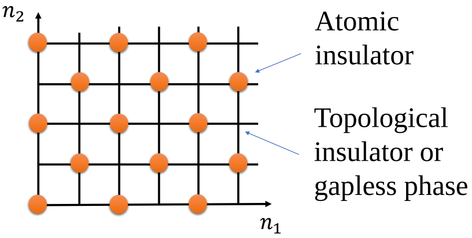
Symmetry indicator Po-Vishwanath-Watanabe

- A diagnostic tool of topological insulators/semimetals from the irreps at high-symmetry points.
- Easy to compute! (cf. generic k-space topological invariants are not classified yet, and they are not easy to compute.)
- Let $n_\alpha^{\boldsymbol{k}} \in \mathbb{Z}_{\geq 0}$ be the number of irrep α at high-symmetry point $\boldsymbol{k}$ $\in$BZ. $\{n_\alpha^{\boldsymbol{k}}\}$ forms a lattice Λ called the band structure.
- The set of atomic insulators (AIs) forms a sublattice $\Lambda_{\mathrm{AI}} \subset \Lambda$.
- Therefore, the complement $\Lambda \backslash \Lambda_{\mathrm{AI}}$ indicates a topological insulator or a gapless phase.



Variants of symmetry indicator

- Symmetry indicator for superconductors. Ono-Watanabe, Ono-Yanase-Watanabe
  - Careful definition of atomic insulators. Skurativska-Neupert-Fischer, KS, Ono-Po-Watanabe, Geier-Brouwer-Trifunovic
- Symmetry indicator for fractional surface/edge/corner charges. Benalcazar-Li-Hughes, Schindler-Brzezińska-Benalcazar-Iraola-Bouhon-Tsirkin-Vergniory-Neupert

Atomic insulator in SCs

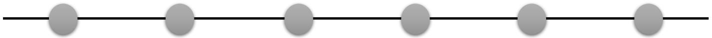
- What are atomic insulators in SCs?
- The many-body setting would helps us to consider this problem.
- Consider a complex fermion $f^\dagger$ as dof.
- We have two ground states: $|0\rangle$ and $f^\dagger |0\rangle$.

- Two states are distinguished by the fermion parity.
- In general, we call $|0\rangle$ of the dof *vacuum*.
- We call the fully occupied state $\prod_j f_j^\dagger |0\rangle$ of the dof the *atomic insulator*.

Symmetry indictor in $1d$

- In 1d with translation invariance, the building-block atomic insulator is the fully occupied state of the dof composed of a complex fermion per unit cell.

$$\prod_{j=1}^{L} f_j^\dagger |0\rangle =$$



- We have the simplest example of the symmetry indicator.
- Atomic insulator for L even must have the trivial fermion parity $(-1)^F = 1$.

$$|\mathrm{AI}\rangle_{L\in\mathrm{even}} \Rightarrow (-1)^F = 1.$$

- Therefore, the negative fermion parity $(-1)^F = -1$ for L even implies the Kitaev chain phase if the state is gapped.

$$|\mathrm{Kitaev}\rangle = f_{k=0}^\dagger \times \prod_{k\neq 0,\pi} (u_k + v_k f_k^\dagger f_{-k}^\dagger) |0\rangle = \left(\sum_i f_i^\dagger + \sum_{i<j<k} f_i^\dagger f_j^\dagger f_k^\dagger + \cdots \right) |0\rangle$$

Symmetry indictor in $2d$

- Similarly, in 2d with translation invariance, atomic insulators must have the trivial fermion parity $(-1)^F = 1$ for even L_x and L_y.

$$|\mathrm{AI}\rangle_{L_x, L_y \in \mathrm{even}} \Rightarrow (-1)^F = 1.$$

- The negative fermion parity $(-1)^F = -1$ for even L_x and L_y implies a topological SC ($(p_x + ip_y)$-wave SC) if the state is gapped. Read-Green

$$|p_x + ip_y\rangle = f^\dagger_{\boldsymbol{k}=\boldsymbol{0}} \times \prod_{\boldsymbol{k} \notin \mathrm{TRIM}} (u_{\boldsymbol{k}} + v_{\boldsymbol{k}} f^\dagger_{\boldsymbol{k}} f^\dagger_{-\boldsymbol{k}}) |0\rangle .$$

BdG Hamiltonian

- A similar symmetry indicator should be defined in free fermions.
- BdG Hamiltonian with translation invariance:

$$\hat{H}_{\mathrm{MF}} = \sum_{\boldsymbol{k}} f_{\boldsymbol{k}}^\dagger h_{\boldsymbol{k}} f_{\boldsymbol{k}} + \frac{1}{2}\sum_{\boldsymbol{k}} f_{\boldsymbol{k}}^\dagger \Delta_{\boldsymbol{k}} (f_{-\boldsymbol{k}}^\dagger)^T + h.c. = \frac{1}{2}(f_{\boldsymbol{k}}^\dagger, f_{-\boldsymbol{k}}) \underbrace{\begin{bmatrix} h_{\boldsymbol{k}} & \Delta_{\boldsymbol{k}} \\ \Delta_{\boldsymbol{k}}^\dagger & -h_{-\boldsymbol{k}}^T \end{bmatrix}}_{=: H_{\boldsymbol{k}}} \begin{pmatrix} f_{\boldsymbol{k}} \\ f_{-\boldsymbol{k}}^\dagger \end{pmatrix}$$

- PHS $\quad CH_{\boldsymbol{k}}C^{-1} = -H_{-\boldsymbol{k}}, \quad C = \tau_x K.$
- We also have the magnetic point group symmetry of $H_{\boldsymbol{k}}$. For unitary symmetry,

$$u_g^{\boldsymbol{k}} \Delta_{\boldsymbol{k}} (u_g^{-\boldsymbol{k}})^T = \xi_g \Delta_{p_g \boldsymbol{k}}, \quad \xi_g \text{ is a 1-dim. rep}$$

$$\Rightarrow \quad \rho_g^{\boldsymbol{k}} H_{\boldsymbol{k}} (\rho_g^{\boldsymbol{k}})^{-1} = H_{p_g \boldsymbol{k}}, \quad \rho_g^{\boldsymbol{k}} = \begin{pmatrix} u_g^{\boldsymbol{k}} & \\ & \xi_g (u_g^{-\boldsymbol{k}})^* \end{pmatrix}.$$

Vacuum and atomic insulators

- In the BdG Hamiltonians, the vacuum and the atomic insulators are written as

$$\hat{H}_{\text{vac}} = \sum_{\boldsymbol{k}} f_{\boldsymbol{k}}^{\dagger} f_{\boldsymbol{k}} \quad \Rightarrow \quad H_{\boldsymbol{k}}^{\text{vac}} = \begin{bmatrix} \mathbf{1} & \\ & -\mathbf{1} \end{bmatrix} = \tau_z,$$

$$\hat{H}_{\text{AI}} = -\sum_{\boldsymbol{k}} f_{\boldsymbol{k}}^{\dagger} f_{\boldsymbol{k}} \quad \Rightarrow \quad H_{\boldsymbol{k}}^{\text{AI}} = \begin{bmatrix} -\mathbf{1} & \\ & \mathbf{1} \end{bmatrix} = -\tau_z.$$

- It should be noticed that the vacuum and the atomic insulator depend on the dof on which the Hamiltonian defined, which we denote it by E_{dof}.

Topological invariants and triple

- Topological invariants of BdG Hamiltonians are designed to determine if two BdG Hamiltonians $H_{\boldsymbol{k}}, H'_{\boldsymbol{k}}$ on the same dof E_{dof} are adiabatically equivalent each other or not.
- We define topological invariants for the triple

$$(E_{\mathrm{dof}}, H_{\boldsymbol{k}}, H'_{\boldsymbol{k}}) \mapsto n(E_{\mathrm{dof}}, H_{\boldsymbol{k}}, H'_{\boldsymbol{k}}) \in \mathbb{Z} \times \mathbb{Z} \times \cdots \times \mathbb{Z}_p \times \cdots$$

- If $H_{\boldsymbol{k}} \sim H'_{\boldsymbol{k}}$ then $n(E_{\mathrm{dof}}, H_{\boldsymbol{k}}, H'_{\boldsymbol{k}}) = 0$.
- The contraposition is important for us. If $n(E_{\mathrm{dof}}, H_{\boldsymbol{k}}, H'_{\boldsymbol{k}}) \neq 0$, then $H_{\boldsymbol{k}} \not\sim H'_{\boldsymbol{k}}$.
- If the set of topological invariants is incomplete to characterize all distinct topological classes, the converse statement is not true. (cf. stable equivalence)

“Irreps” at high-symmetry points

- As in the case of insulators, irreps of high-symmetry points are computable topological invariants for SCs.
- On TRIMs Γ, according to how PHS acts on each irrep at Γ, which can be computed by the Wigner criteria for TRS and PHS, we have a nontrivial $\mathbb{Z}$ or $\mathbb{Z}_2$ topological invariant, or no topological invariants.

$\mathbb{Z}_2$ and $\mathbb{Z}$ invariants

- (For simplicity, we assume no TRS.)
- When PHS operator preserves an irrep α at a TRIM Γ, we have a $\mathbb{Z}_2$ Pfaffian invariant

$$\nu_\Gamma^\alpha(E_{\mathrm{dof}}, H_{\boldsymbol{k}}, H'_{\boldsymbol{k}}) = \frac{1}{\pi}\mathrm{Arg}\left[\frac{\mathrm{Pf}\left[H_\Gamma \tau_x\right]}{\mathrm{Pf}\left[H'_\Gamma \tau_x\right]}\right] \in \mathbb{Z}_2 = \{0, 1\}.$$

- When PHS operator exchanges irreps α and β at a TRIM Γ, we have the $\mathbb{Z}$ invariant as the number of irreps

$$n_\Gamma^\alpha(E_{\mathrm{dof}}, H_{\boldsymbol{k}}, H'_{\boldsymbol{k}}) = N_\alpha[H_\Gamma] - N_\alpha[H'_\Gamma] \in \mathbb{Z},$$

where $N_\alpha[H]$ is the number of α-irrep for the occupied states of H.

- (These expressions become simplified in the weak coupling limit.)

Symmetry indicator for SCs

- We define the band structure Λ as a lattice of $\mathbb{Z}$ and $\mathbb{Z}_2$ topological invariants at high-symmetry points.
- We define the subset $\Lambda_{\mathrm{AI}} \subset \Lambda$ generated by the $\mathbb{Z}$ and $\mathbb{Z}_2$ topological invariants of the triples of atomic insulators relative to the vacuum

$$(E_{\mathrm{dof}}, H_{\boldsymbol{k}}^{\mathrm{AI}}, H_{\boldsymbol{k}}^{\mathrm{vac}}) = (E_{\mathrm{dof}}, -\tau_z, \tau_z).$$

- The symmetry indictor for SCs is defined as the complement

$$\Lambda \backslash \Lambda_{\mathrm{AI}}.$$

- $(E_{\mathrm{dof}}, H_{\boldsymbol{k}}, H_{\boldsymbol{k}}^{\mathrm{vac}}) \notin \Lambda_{\mathrm{AI}}$ implies that $H_{\boldsymbol{k}}$ is not an atomic insulator, i.e., a topological SC or a gapless SC.

Ex: d-dim., PHS only,

- Consider a d-dim lattice with PHS only.
- The band structure is

$$\Lambda = \mathbb{Z}_2^{\times(N-1)},$$

where N is the number of TRIMs.
- There is one generator atomic insulator.

$$\Lambda_{\mathrm{AI}} = \mathbb{Z}_2.$$

- The symmetry indicator is classified as

$$\Lambda/\Lambda_{\mathrm{AI}} = \mathbb{Z}_2^{\times(N-2)}.$$

- This reproduces the many-body symmetry indicator by the fermion parity.

Ex: P$\bar{1}$, odd parity SC

- Consider the $3d$ space group P$\bar{1}$ and odd parity SCs $I_{\boldsymbol{k}} \Delta_{\boldsymbol{k}} I^T_{-\boldsymbol{k}} = -\Delta_{-\boldsymbol{k}}$.
- The lattice Λ of the band structure is $\mathbb{Z}^{\times 8}$ composed of $\mathbb{Z}$ invariants for TRIMs

$$n_{\Gamma_j}(E_{\rm dof}, H_{\boldsymbol{k}}, H'_{\boldsymbol{k}}) = N_{I_{\rm BdG}=1}[H_{\Gamma_j}] - N_{I_{\rm BdG}=1}[H'_{\Gamma_j}].$$

- The symmetry indicator is classified as

$$\Lambda/\Lambda_{\rm AI} = \mathbb{Z}_8 \times \mathbb{Z}_4^{\times 3} \times \mathbb{Z}_2^{\times 3}.$$

- The $\mathbb{Z}_8$ indicator defined by

$$z := \sum_{\Gamma_j \in \{\Gamma, U, V, T\}} n_{\Gamma_j} - \sum_{\Gamma_j \in \{X, Y, Z, R\}} n_{\Gamma_j} \in \mathbb{Z}/8\mathbb{Z}$$

indicates

$z = 1$ Weyl SC,
$z = 2$ 2nd-order SC,
$z = 4$ 3rd-order SC.

Summary

- We proposed the construction of the symmetry indicator for SCs.
- The band structure $=\mathbb{Z}$ and $\mathbb{Z}_2$ invariants at high-symmetry points.
- Topological invariants are defined for the triple

$$(E_{\rm dof}, H_{\boldsymbol{k}}, H'_{\boldsymbol{k}}).$$

- The subset $\Lambda_{\rm AI} \subset \Lambda$ of the atomic insulators is defined by the triples

$$(E_{\rm dof}, H^{\rm AI}_{\boldsymbol{k}}, H^{\rm vac}_{\boldsymbol{k}}).$$

- $(E_{\rm dof}, H_{\boldsymbol{k}}, H^{\rm vac}_{\boldsymbol{k}}) \notin \Lambda_{\rm AI}$ implies that $H_{\boldsymbol{k}}$ is a topological SC or a gapless SC.

- Back Up

$\mathbb{Z}_2$ and $\mathbb{Z}$ invariants (cont.)

- These $\mathbb{Z}_2$ and $\mathbb{Z}$ invariants are invariants of the K-theory.
- Stable equivalence

$$n_{\Gamma}^{\alpha}(E_{\text{dof}} \oplus E'_{\text{dof}}, H_{\boldsymbol{k}} \oplus H''_{\boldsymbol{k}}, H'_{\boldsymbol{k}} \oplus H''_{\boldsymbol{k}}) = n_{\Gamma}^{\alpha}(E_{\text{dof}}, H_{\boldsymbol{k}}, H'_{\boldsymbol{k}}),$$

- Therefore, topologically inequivalent pair $H_{\boldsymbol{k}} \not\sim H'_{\boldsymbol{k}}$ may give the same
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$$-n_{\Gamma}^{\alpha}(E_{\text{dof}}, H_{\boldsymbol{k}}, H'_{\boldsymbol{k}}) = n_{\Gamma}^{\alpha}(E_{\text{dof}}, H'_{\boldsymbol{k}}, H_{\boldsymbol{k}}).$$